Phase transition in a two-dimensional Ising ferromagnet based on the generalized zero-temperature Glauber dynamics

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(Received 18 March 2013; revised manuscript received 28 April 2013)

At zero temperature, based on the Ising model, the phase transition in a two-dimensional square lattice is studied using the generalized zero-temperature Glauber dynamics. Using Monte Carlo (MC) renormalization group methods, the static critical exponents and the dynamic exponent are studied; the type of phase transition is found to be of the first order.

Keywords: zero-temperature Glauber dynamics, phase transition, Monte Carlo renormalization group

PACS: 75.10.Hk, 75.40.Mg, 05.10.Cc, 64.60.Ht **DOI:** 10.1088/1674-1056/22/12/127501

1. Introduction

In recent years, lots of theoretical studies have been carried out on the zero-temperature phase transition, pointing out that even at the zero temperature, other factors can determine the phase transition, such as the pressure, the density, the magnetic field, etc.[1–5] Besides, the type of zero-temperature phase transition is usually of the first order. Although the zero-temperature phase transition is usually attributed to the quantum effect, it can sometimes be dealt with by using classical methods.[6] The Glauber dynamics[7] is one of the classical spin dynamic methods, which is used to study critical dynamics. With the temperature coming to zero, it becomes the zero-temperature Glauber dynamics, which has attracted a great deal of attention in recent years.

The original zero-temperature Glauber dynamics in an Ising ferremagnet can be summarized as follows. Choose a spin from the system at random at each timestep, and let it do spin flipping. If the sum of neighboring spins is greater than zero, the spin after flipping will take the value +1. If the sum is lower than zero, the spin after flipping will take the value -1. Otherwise, the spin after flipping has an equal probability to take the value +1 or -1. Based on the original zero-temperature dynamics, many interesting results are found. For example, in a one-dimensional (1D) chain, under that dynamics, the system will always reach the ground state, i.e., all spins take the same value.[8] In a two-dimensional (2D) square lattice, the system has only about a $1/3$ probability to reach the ground state.[9,10] While in a three-dimensional (3D) cubic lattice, the system will never reach the ground state,[11] because of the existence of blinkers. Besides, for the zero-temperature Glauber dynamics in complex networks, in the thermodynamic limit, the systems will never reach the ground state.[12–15] So for different types of systems, whether the systems will reach the ground state, the dimension of the system plays a key role.

Later, a generalized zero-temperature Glauber dynamics containing a tunable parameter is proposed. The phase transition at zero temperature can be studied both theoretically and numerically.[16] Under generalized zero-temperature Glauber dynamics, for Ising spins, each spin is flipped $\sigma_i(t) \to -\sigma_i(t+1)$ with a rate $W(\delta E)$ at each timestep. The rate is defined as

$$W(\delta E) = \begin{cases} 1, & \text{if } \delta E < 0, \\ W_0, & \text{if } \delta E = 0, \\ 0, & \text{if } \delta E > 0, \end{cases} \tag{1}$$

where δE denotes the energy difference and W_0 represents the spin flipping probability of $\sigma_i(t) \to -\sigma_i(t+1)$ with $\delta E = 0$.

Using the generalized zero-temperature Glauber dynamics, the study was carried out in a 1D Ising ferromagnet with a synchronous updating mode. A phase transition was observed, which was found to be of a continuous nature, and the critical exponents were found to be $\beta \approx 0, \nu \approx 1, z \approx 2$.[17]

We have carried out the study in a 2D Ising ferromagnet using that dynamics with the synchronous updating mode, but found no phase transition in the system; while the use of that dynamics with a random updating mode in the 2D Ising ferromagnet has already been carried out.[18] It was found that there was no phase transition but an absorbing state. So we try to further generalize that dynamics, and the further generalized dynamics is introduced as follows. The rate $W(\delta E)$ is modified as

$$W(\delta E) = \begin{cases} 1, & \text{if } \delta E < 0, \\ W_0 \text{ or } 1-W_0, & \text{if } \delta E = 0, \\ 0, & \text{if } \delta E > 0, \end{cases} \tag{2}$$

where W_0 denotes the probability of $\sigma(t) \to \sigma_i(t+1) = 1$, so $1 - W_0$ represents the probability of $\sigma(t) \to \sigma_i(t+1) = -1$. Obviously, if $W_0 = 0.5$, the dynamics will come back to the original zero-temperature Glauber dynamics.

The interest in zero-temperature Glauber dynamics has been aroused partially by recent experiments with single-chain

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magnets,[19] but it is also due to the development of non-equilibrium statistical physics. At zero temperature, even after a spin flipping, with the energy difference satisfying $\delta E = 0$, we assume the spin after flipping might tend to take one value other than the other. So with $\delta E = 0$, the spin flipping probability W_0 might take the value from 0 to 1 continuously, if the system is controlled by several factors (the pressure, the density, the magnetic field, etc.) simultaneously.[1–5]

Besides, using our proposed dynamics, we carried out the research in a 2D Ising ferromagnet using a sequential spin updating mode. We name our proposed dynamics the generalized zero-temperature Glauber dynamics and found a phase transition in the system. For the studies, at first, we determined the critical point of the phase transition with the generalized specific heat $C(W_0)$ and the generalized susceptibility $\chi(W_0)$. Then, we found the values of static critical exponents with the Monte Carlo renormalization group (MCRG) method. Next, we determine the value of the dynamic exponent z with the dynamic Monte Carlo renormalization group (DMCRG) method. Finally, according to the values of critical exponents and the behavior of the generalized order parameter $m(W_0)$ near the critical point, we regard the type of phase transition as of the first order.

The rest of this paper is organized as follows. In Section 2, the static critical exponents are studied with the MCRG method, and verified by the best data collapse method. In Section 3, the dynamic exponent is studied with the DMCRG method. Finally, in Section 4, some conclusions are drawn from this study.

2. Static critical exponents

We generalize the MCRG method proposed by Swendsen[20] and use it to find the values of the static critical exponents. The studies are carried out in a 2D square lattice of Ising spins. For the 2D Ising ferromagnet, the periodic boundary condition is satisfied. The size of the lattice is denoted as N, and the length is represented by L. As in Ref. [20], the renormalized Hamiltonian of the system is defined as

$$H = \sum_{\alpha} K_{\alpha} S_{\alpha}. \tag{3}$$

Here, S_α is some combination of the σ's. For example,

$$S_1 = \sum_{\langle i,j \rangle} \sigma_i \sigma_j, \tag{4}$$

where the sum $\sum_{\langle i,j \rangle}$ runs over all the nearest neighbors. In the vicinity of the fixed-point Hamiltonian, H^*, the following relations are assumed to be[21]

$$K_{\alpha}^{(n+1)} - K_{\alpha}^{*} = \sum_{\beta} T_{\alpha\beta}^{*} (K_{\beta}^{(n)} - K_{\beta}^{*}), \tag{5}$$

where

$$T_{\alpha\beta}^{*} = [\partial K_{\alpha}^{(n+1)} / \partial K_{\beta}^{(n)}]_{H^*}, \tag{6}$$

the eigenvalue equation can be expressed as

$$\sum_{\alpha} \varphi_{\alpha} T_{\alpha\beta}^{*} = \lambda \varphi_{\beta}. \tag{7}$$

The critical exponents are obtained in the usual way to be $\nu = \ln b / \ln \lambda_1^{\mathrm{e}}$ and $\eta = d + 2 - 2 \ln \lambda_1^{\mathrm{o}} / \ln b$, where $\lambda_1^{\mathrm{e(o)}}$ is the largest even (odd) eigenvalue.

Although at the zero-temperature, the temperature no longer plays an important role, we propose that the spin flipping probability W_0 could play the role of temperature T. So we use W_0 to substitute for T, which means that the MCRG method can be used based on the spin flipping mechanism, as shown in Eq. (2).

Firstly, we try to determine the critical value of spin flipping probability W_{c} at which the phase transition will take place. We assume the critical value to be $W_{\mathrm{c}} = 0.5$. It is verified by the numerical results of the generalized specific heat $C(W_0)$ and the generalized susceptibility $\chi(W_0)$, which are originally used in the equilibrium process. Although at the zero temperature, the ensemble average of the system no longer equals the time average, because the ergodicity is broken, the system will reach a dynamic balance state after a long enough time. So we assume that those generalized thermodynamic functions $C(W_0)$ and $\chi(W_0)$ are still useful in the nonequilibrium process to determine the critical value W_{c}, as they show a sharp peak at the critical value W_{c} in a finite-size system. The generalized specific heat $C(W_0)$, the generalized susceptibility $\chi(W_0)$, and the generalized order parameter $m(W_0)$ are expressed as follows:

$$C(W_0) = W_0^2 (\langle E^2 \rangle - \langle E \rangle^2)/N, \tag{8}$$

$$\chi(W_0) = W_0 N (\langle m^2 \rangle - \langle |m| \rangle^2), \tag{9}$$

$$m(W_0) = \langle m \rangle = \left\langle \frac{1}{N} \sum_i \sigma_i \right\rangle, \tag{10}$$

and

$$E = -\sum_{\langle i,j \rangle} \sigma_i \sigma_j, \tag{11}$$

where the sum $\sum_{\langle i,j \rangle}$ runs over all the nearest spins. The critical value is verified to be $W_{\mathrm{c}} = 0.5$, as shown by the numerical results in Fig. 1.

Next, in the 2D Ising ferromagnet, we divide the square lattice into 3×3 blocks (scale factor $b = 3$). Each block takes a spin +1 or -1 by majority rule. We use the MCRG method in two lattices of sizes 81×81 and 243×243. In the simulation, we consider up to two even interactions (nearest-neighbor, second-neighbor) and one odd interaction (magnetic field). The numerical results of the exponents are shown in Table 1.

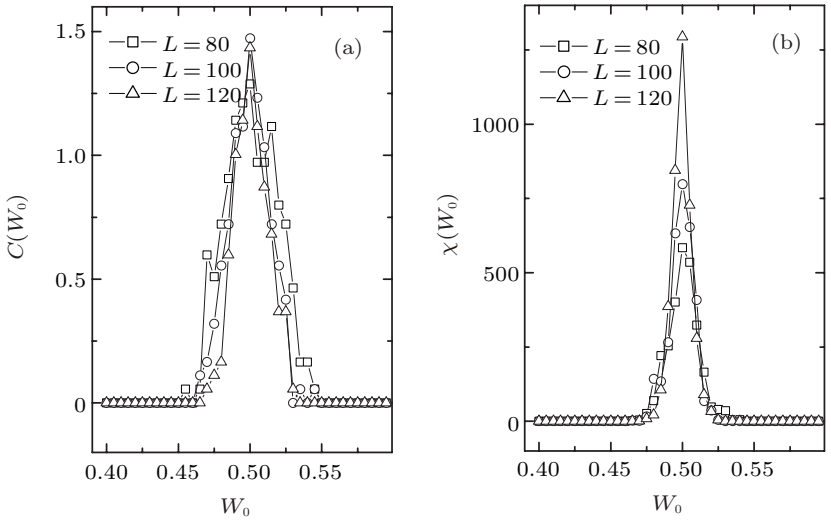


Fig. 1. (a) Curves of generalized specific heat $C(W_0)$ and (b) the generalized susceptibility $\chi(W_0)$. The lengths of the 2D square lattice are $L = 80$, $L = 100$, and $L = 120$. There are 10^5 spin flips over each spin, and the numerical results are the values averaged over 100 realizations. If $L \to \infty$, then $C(W_0)$ and $\chi(W_0)$ will diverge at $W_c = 0.5$. Because of the finite-size effect, $C(W_0)$ and $\chi(W_0)$ only take finite values at the critical value W_c respectively.

Table 1. Eigenvalues and critical exponents obtained from the MCRG method of a 2D Ising model using two lattices of sizes 81×81 and 243×243 with 10^6 MC timesteps/site. In the Table, L denotes the length of the lattice, n the iteration number, and m the number of even interactions.

	n	m	λ_1^e	α	ν	λ_1^o	δ	η	β	γ
$L = 81$	1	1	3.000	0.000	1.000	9.015		−0.003052	−0.001526	2.003
		2	3.000	0.000	1.000				0.000	2.000
	2	1	3.000	0.000	1.000	8.938		0.01260	0.006303	1.994
$L = 243$	1	1	3.000	0.000	1.000	8.998		0.0003237	0.0001618	2.000
		2	3.000	0.000	1.000				0.000	2.000
	2	1	3.000	0.000	1.000	9.000		0.000	0.000	2.000
Average			3.0	0	1.0	8.988		0.002468	0.0008231	2.0

Finally, we obtain the average values of the critical exponents to be $\alpha = 0$, $\nu = 1.0$, $\eta = 0.002468$, $\beta = 0.0008231$, $\gamma = 2.0$, and $\delta \to \infty$ with $L \to \infty$. We use the best data collapse method to verify the correctness of the critical exponents α, β, γ, and ν. The scaling form of the generalized magnetization $m(\tau, L)$, the generalized specific heat $C(\tau, L)$, and the generalized susceptibility $\chi(\tau, L)$ are expressed as follows:

$$m(\tau, L) \sim L^{-\beta/\nu} f_1(\tau L^{1/\nu}), \tag{12}$$

$$C(\tau, L) \sim W_0 L^{\alpha/\nu} f_2(\tau L^{1/\nu}), \tag{13}$$

$$\chi(\tau, L) \sim L^{\gamma/\nu} f_3(\tau L^{1/\nu}), \tag{14}$$

where $\tau = 1 - W_0/W_c$, and f_1, f_2, f_3 are associated functions.

The numerical results of the best data collapse are shown in Figs. 2–4. Besides, based on Fig. 2, the critical exponent $\beta \approx 0$, if $L \to \infty$ then $\beta \to 0$. Along with considering the relation $m(W_0) \sim \tau^\beta$ in an infinite-size system, the generalized

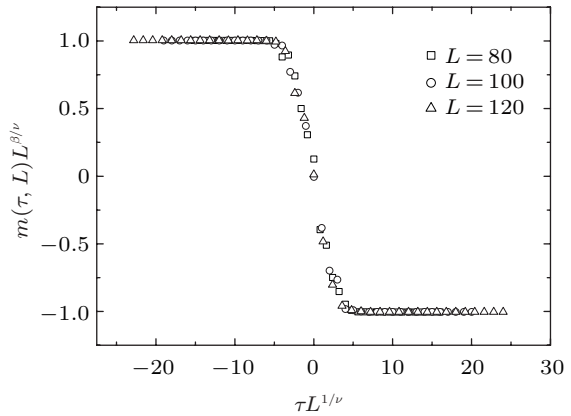


Fig. 2. Variations of $m(\tau, L)L^{\beta/\nu}$ with $\tau L^{1/\nu}$, with $\beta \approx 0, \nu = 1.0$, and lengths of the lattices $L = 80$, 100, 120. There are 10^5 spin flips over each spin from random initial conditions. The results are the values averaged over 100 realizations.

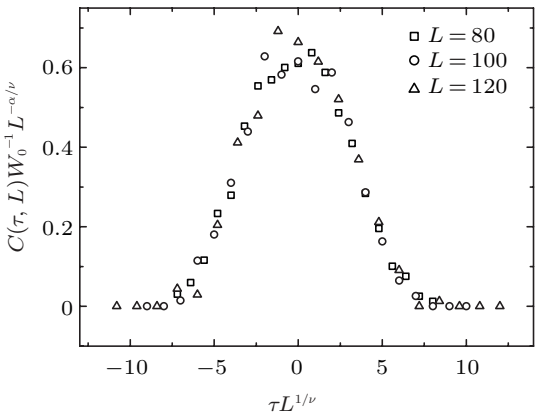


Fig. 3. Variations of $C(\tau, L)W_0^{-1}L^{-\alpha/\nu}$ with $\tau L^{1/\nu}$, with $\alpha = 0$ and $\nu = 1.0$. There are 10^5 spin flips over each spin from random initial conditions. The results are the values averaged over 200 realizations.

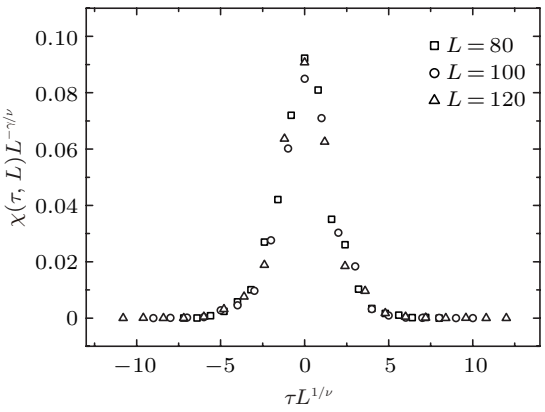


Fig. 4. Variations of $\chi(\tau,L)L^{-\gamma/\nu}$ with $\tau L^{1/\nu}$, with $\gamma=2.0$, $\nu=1.0$. There are 10^5 spin flips over each spin from random initial conditions. The results are the values averaged over 200 realizations.

magnetization $m(W_c)$ will change from +1 (−1) to −1 (+1) suddenly with $L\to\infty$. From those considerations, we consider the type of phase transition to be of the first order and the phase transition to be of a continuous nature in a finite-size system.

3. Dynamic critical exponent

In this section, we try to find the dynamic exponent z using the DMCRG method.[22,23] The dynamic exponent is determined with the correlation functions, such as

$$E(N,n,W_{02};t)=E'(Nb^d,n+1,W_{01};b^z t), \tag{15}$$

and

$$C(N,n,W_{02};t)=C'(Nb^d,n+1,W_{01};b^z t), \tag{16}$$

where

$$E(N,n,W_0;t)=(N^{(n)})^{-1}\left\langle\sum_{\langle i,j\rangle}S_i^{(n)}(t)S_j^{(n)}(0)\right\rangle_{W_0,N}, \tag{17}$$

and

$$C(N,n,W_0;t)=(N^{(n)})^{-1}\left\langle\sum_{i}S_i^{(n)}(t)S_i^{(n)}(0)\right\rangle_{W_0,N}. \tag{18}$$

In the correlation functions, we have replaced the temperature with the spin flipping probability W_0. Besides, N denotes the size of the system, n the iteration number, b the scale of spin blocks, d the dimension of the system, and t the timestep. We choose $W_{01}=W_{02}=W_c$ for the convenience of simulation, where $W_c=0.5$ is the critical value of an infinite-size system.

For two different sizes of systems, we set the initial values of the correlation functions to be equal to each other, which are as follows:

$$E(N,n,W_c;0)=E'(Nb^d,n+1,W_c;0), \tag{19}$$

and

$$C(N,n,W_c;0)=C'(Nb^d,n+1,W_c;0), \tag{20}$$

where E' and C' denote the correlation functions of the larger systems. From random initial conditions, using the DMCRG method, after a long enough time, we find the relations of $E(t)\sim t^{-\gamma}, E'(t')\sim t'^{-\gamma}$, $C(t)\sim t^{-\gamma}$, and $C'(t')\sim t'^{-\gamma}$. Considering the relation $t'=tb^z$, we can obtain the dynamic exponent z from the following relations:

$$z\simeq\frac{\ln E'(t)-\ln E(t)}{\gamma\ln b}, \tag{21}$$

and

$$z\simeq\frac{\ln C'(t)-\ln C(t)}{\gamma\ln b}, \tag{22}$$

where γ can be obtained from the distribution of $E(t)$ varying with t, etc., which are shown in Fig. 5 for example.

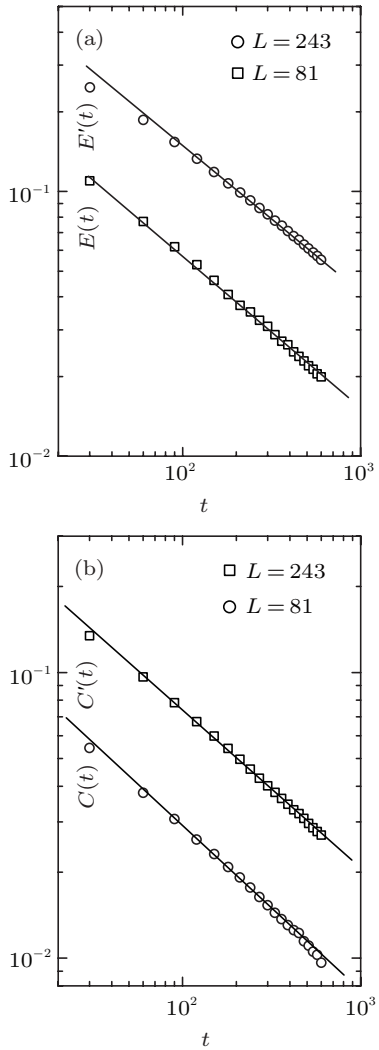


Fig. 5. Variations of $E(t)$ and $E'(t)$ (a) and $C(t)$ and $C'(t)$ (b) with t. $E'(t)$ and $C'(t)$ are the correlation functions of the larger lattice of size 243×243 after one iteration, while $E(t)$ and $C(t)$ are the functions of the smaller lattice of size 81×81. The numerical results are the values averaged over 10^3 realizations. From this figure, we can obtain the values of $\ln E'(t)-\ln E(t)$, $\ln C'(t)-\ln C(t)$, and the value of γ.

To find the dynamic exponent z, we use the DMCRG method in two square lattices of sizes 243×243 and 81×81. The scale of spin blocks is chosen to be $b=3$. The values of

$\ln E'(t) - \ln E(t)$, $\ln C'(t) - \ln C(t)$, and γ can be obtained from the distributions of $E(t)$, $E'(t)$, etc. We have found that the value of γ ranges from 0.4927 to 0.5654. Finally, we find the average value of the dynamic exponent to be $z = 1.51 \pm 0.05$, which is shown in Table 2.

Table 2. In this Table, L denotes the length of the larger lattice, and n the iteration number of the larger lattice. The size of the smaller lattice is L/b, and the iteration number of the smaller lattice is $n-1$ accordingly. $E'(t)$ and $C'(t)$ are the correlation functions of the larger lattice. The values of z are calculated from Eqs. (21) and (22) based on the numerical results as shown in Fig. 5 for example.

	$E'(t)$	z	$C'(t)$	z	Average
$L = 243$	n=1	1.58	n=1	1.56	1.57
	n=2	1.47	n=2	1.42	1.45
$L = 81$	n=1	1.55	n=1	1.50	1.53
Average		1.53		1.49	1.51± 0.05

Because $E(t)$ and $C(t)$ are different correlation functions, and for different sizes of two lattices and different iteration numbers, the values of z are in a reasonable domain, so we consider the average value of the dynamic exponent $z = 1.51 \pm 0.05$ to be acceptable.

4. Conclusions

We try to establish zero-temperature dynamics to describe the zero-temperature phase transition. We take the type of phase transition at zero temperature to be of the first order. We name our established zero-temperature dynamics the generalized zero-temperature Glauber dynamics. Firstly, we carry out the generalized zero-temperature Glauber dynamics in the 2D Ising ferromagnet. Using the MCRG method, we obtain the values of the static critical exponents, such as α, β, γ, ν, etc. Secondly, using the DNMRG method, we obtain the value of the dynamic critical exponent to be $z = 1.51 \pm 0.05$. Thirdly, considering that the critical exponent $\beta \approx 0$, and $\beta \to 0$ with $L \to \infty$, the generalized magnetization $m(W_c)$ will change from $+1$ (-1) to -1 $(+1)$ suddenly with $L \to \infty$. Finally, based on those considerations, we consider the type of phase transition under the generalized zero-temperature Glauber dynamics to be of the first order.

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